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Temperature Dependence of Band Gaps in Semiconductors: Electron-Phonon Interaction J.S. BHOSALE, A.K. RAMDAS, Purdue University, West Lafayette, IN, USA, A. BURGER, Fisk University, Nashville, TN, USA, A. MUÑOZ, Universidad de La Laguna, Tenerife, Spain, A.H. ROMERO, Max Planck Institut, Halle, Germany, M. CARDONA, R. LAUCK, R.K. KREMER, Max Planck Institut, Stuttgart, Germany — A theoretical investigation with *ab initio* techniques of the electron-phonon interaction of semiconductors with chalcopyrite structure and its comparison with modulated reflectivity experiments yield a striking difference between those with ($AgGaS_2$) and without ($ZnSnAs_2$) d electrons in their valence bands. The former exhibit a non-monotonic temperature dependence of the band gaps whose origin is not yet fully understood. The analysis of this temperature dependence with the Bose-Einstein oscillator model[1] involving two oscillator terms having weights of opposite signs, provides an excellent agreement with the experimental data and correlates well with the characteristic peaks in the phonon density of states associated with the acoustical phonon modes. This work underscores the need for theoretical understanding of the electron-phonon interaction involving d electrons, particularly in *ab initio* investigations.

[1]Göbel *et. al.* Phys. Rev. B 57, 15183 (1998).

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