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Structure and dynamics of a Ag-doped chalcogenide glass: an *ab initio* study[1] DALE IGRAM, HORACIO CASTILLO, DAVID DRABOLD, Ohio University — The vibrational properties of a ternary glassy chalcogenide material, $Ag_{20}Ge_{28}Se_{52}$, are analyzed. The vibrational density of states and atomic participation ratios calculations revealed that Se atoms are a major contributor across the vibrational spectrum. The abrupt change and plateau of the stretching character may be due to vibrational contribution changes and a difference in the rate of change for the Ge and Se atoms, respectively. The divergence of the perpendicular phase quotient is due to the rocking motion of a Ge-Ge compound. A1 breathing modes of the corner-sharing tetrahedra showed that these breathing modes are non-local and involve the mixing of modes of different symmetry resulting in two bands of A1 breathing modes.

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