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First principles determination of vibrational and elastic properties of quaternary compounds Cu_2ZnSnS_4 and $Cu_2ZnSnSe_4$ TANJU GUREL, CEM SEVIK, TAHIR CAGIN, Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX — Recently, the quaternary compounds, Cu_2ZnSnS_4 and $Cu_2ZnSnSe_4$, have been attracted pretty much attention because of their potential use in the field of energy harvesting applications. Several theoretical calculations have been reported about their first principles electronic, optic and transport properties. However, no lattice dynamic calculations have been published yet despite the discussions about their possible ground state crystal structures and measured low thermal conductivity values. In this systematical study, we examined the vibrational and elastic properties of the two different crystal phases, kesterite (KS) with space group $I\bar{4}$ and stannite (ST) with space group $I\bar{4}2m$, of this quaternary compounds by using density functional perturbation theory. In addition, we predicted the relaxation time dependent lattice thermal conductivity within the solution of phonon Boltzmann transport equation by making use of the acquired vibrational frequency data.

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