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Computational Study of the Vibrational, Thermal and Transport Properties of the Type II Tin Clathrate Compounds Cs_xSn_{136} (x = 12, 16, 20) DONG XUE, CHARLES MYLES, Texas Tech University — The Type II clathrates A_xB_{136} (A = alkali atom; B = Si, Ge, Sn) are interesting because of their low lattice thermal conductivity and thermoelectric properties. Their low thermal conductivity is due to the low-frequency vibrational modes produced by the alkali guests in the host lattice cages. Heat transport theory predicts that such modes will scatter with the acoustic phonons of the host, reducing the lattice thermal conductivity. To understand this effect for the Type II Sn clathrates, we have performed a first principles computational study of the vibrational, thermal, and transport properties of Cs_xSn_{136} (x = 12,16,20). Our calculations use the VASP and PHONOPY codes to calculate the vibrational modes. We present results for the phonon modes, the heat capacity, and the Gruneisen parameter in Cs_xSn_{136}. Our calculated Cs modes are in the range 8-15 cm^{-1} and we find that these frequencies decrease as x increases. Our results for the vibrational contribution to the heat capacity predict that it weakly depends on x, and that it increases smoothly with temperature T, approaching the Dulong-Petit value at T = 600 K. Our calculations of the Gruneisen parameter predict that it has a weak x dependence, it increases with increasing T for 160 K $\leq$ T $\leq$ 300 K and it has a weak dependence on T for 300 K $\leq$ T $\leq$ 550 K. We have used these results to calculate the lattice thermal conductivity in Cs_xSn_{136} within the kinetic theory approximation. The results of these calculations are also presented and discussed.

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