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First principles calculations of the thermal properties of tin clathrate materials EMMANUEL NENGHABI, Texas Tech Univeristy, CHARLES MYLES, Texas Tech University — Using a Local Density Approximation (LDA) approach, we have studied the energetics and the thermal properties (free energy, specific heat, lattice vibrational entropy) of the tin-based Type I semiconductor clathrates Sn_{46}, K_8Sn_{46}, $K_8Sn_{44}M_2$ (M is a Sn vacancy), $Cs_8Ga_8Sn_{38}$ and $Cs_8Zn_4Sn_{42}$. The clathrate lattices are open framework, cage-like structures. Our results predict that K_8Sn_{46} is slightly less stable than $K_8Sn_{44}M_2$, in agreement with other theories.[1] We have optimized the geometry of each structure and have calculated the phonon density of states. The thermodynamic properties have then been calculated as a function of temperature. The localized vibrational ("rattler") modes of the guests Cs and K have been calculated and their Einstein temperatures obtained. The Debye temperatures of each host clathrate have also been calculated. We use our results to help to explain the observed difference[2] in the lattice thermal conductivities of some of these materials.

[1]L. Mollnitz et. al., J. Chem. Phys. 117, 3 (2002)
[2]G. S. Nolas et. al., Phys. Rev. B 53,165201 (2002)

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