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Effects of silicon on the vibrational and thermal properties of the clathrates $\mathbf{A_8Ga_{16}Si_xGe_{30-x}}$ (A= Ba, Sr) CHARLES MYLES, Texas Tech Univeristy, EMMANUEL NENGHABI, Texas Tech University — Using the GGA, we have calculated the vibrational and thermal properties of the clathrates $Ba_8Ga_{16}Si_xGe_{30-x}$ and $Sr_8Ga_{16}Si_xGe_{30-x}$ for x = 0, 5 and 15. We find that the Ba and Sr guests have localized vibrational modes lying below 80 cm^{-1}, which tend to reduce the host acoustic bandwidth. We predict that there is an upshift in the framework optic modes as x increases and that the guest-atom Einstein temperatures vary with x. Our predicted isotropic atomic displacement parameters as functions of temperature for the Ba and Sr guests in these clathrates show that Sr has a larger isotropic displacement parameter than Ba, suggesting that Sr should be more efficient than Ba in lowering the thermal conductivity. We also predict the temperature dependences of the vibrational specific heat, the entropy, and the Helmholtz free energy in these materials. We find that the specific heat increases smoothly with temperature and approaches the Dulong-Petit value at room temperature. We also find that there is a slight x dependence of the heat capacity, free energy, and vibrational entropy.

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