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Theoretical study of thermal properties of Si clathrates[1] XIAOLI TANG, JIANJUN DONG, Physics Department, Auburn University — Pristine silicon clathrate (Si_{136}) is an "expanded volume" allotrope of Si that is metastably available at ambient conditions, and it exhibits a significant decrease in lattice thermal conductivity. We have theoretical studied vibrational, thermodynamic, and transport properties of Si_{136} and compared its results with those of the ground state diamond-structured Si. The equilibrium temperature-pressure phase boundary between the two phases occurs in the negative pressure regime. Despite obvious differences in the energetics and lattice vibrational modes for the two polymorphic forms of Si, our calculations indicate that their heat capacities are quite similar. We further predict that Si_{136} has a region of negative thermal expansion below T=140K. Our *ab initio* prediction shows that thermal expansion in the guest-free Si_{136} clathrate is significantly smaller than the previously reported data of guest encapsulated clathrates. In contrast to similar thermal properties in the two phases, our calculations of lattice thermal conductivities reveal some dramatically different features in the phases. We will discuss the origin of the predicted "oscillation" in the current-current correlation functions.

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