Properties of the type I Ge-based clathrates Ba$_8$Al$_{13}$Ge$_{33}$ and Ba$_8$Al$_{16}$Ge$_{30}$

EMMANUEL NENGHABI, Texas Tech University, CHARLES MYLES, Texas Tech University — The type I clathrate lattice is simple cubic with 46 atoms per unit cell. The cages in this lattice can host “guests” and the framework can have substituted atoms. Here, we focus on the “alloy” system Ba$_8$Al$_x$Ge$_{30}$−$_x$ (x is an integer; 0<x<15). The Ba are guests and Al substitutes for some Ge framework atoms. Using the local density approximation (LDA), we have calculated some properties of the type I clathrates Ba$_8$Al$_{13}$Ge$_{33}$ and Ba$_8$Al$_{16}$Ge$_{30}$. Our calculations of the equilibrium structures predict that Ba$_8$Al$_{16}$Ge$_{30}$ and Ba$_8$Al$_{13}$Ge$_{33}$ have approximately the same lattice constant and that Ba$_8$Al$_{13}$Ge$_{33}$ is expected to be slightly more stable than Ba$_8$Al$_{16}$Ge$_{30}$. Our band structures and electronic density of states results predict that Ba$_8$Al$_{13}$Ge$_{33}$ is metallic and that Ba$_8$Al$_{16}$Ge$_{30}$ is a semiconductor with an indirect fundamental band gap of 0.3 eV. The vibrational spectrum predicts low frequency rattling modes caused by the Ba guests that are loosely bound in the Al-Ge framework cages. Such modes may scatter the heat-carrying acoustic vibrational framework modes, potentially reducing the thermal conductivity.

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