Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Properties of the type I Ge-based clathrates $Ba_8Al_{13}Ge_{33}$ and $Ba_8Al_{16}Ge_{30}$ EMMANUEL NENGHABI, Texas Tech Univeristy, 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 $Ba_8Al_xGe_{30-x}$ (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 $Ba_8Al_{13}Ge_{33}$ and $Ba_8Al_{16}Ge_{30}$. Our calculations of the equilibrium structures predict that $Ba_8Al_{16}Ge_{30}$and $Ba_8Al_{13}Ge_{33}$ have approximately the same lattice constant and that $Ba_8Al_{13}Ge_{33}$ is expected to be slightly more stable than $Ba_8Al_{16}Ge_{30}$. Our band structures and electronic density of states results predict that $Ba_8Al_{13}Ge_{33}$ is metallic and that $Ba_8Al_{16}Ge_{30}$ 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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Date submitted: 03 Dec 2007 Electronic form version 1.4