

Abstract Submitted
for the TSS07 Meeting of
The American Physical Society

Electronic and vibrational properties of the clathrate “alloy” $\text{Ba}_8\text{Ga}_{16}\text{Ge}_{30-x}\text{Si}_x$ EMMANUEL NENGHABI, Texas Tech Univeristy, CHARLES MYLES, Texas Tech University — We have used the Generalized Gradient Approximation (GGA) of density functional theory (DFT) to study the electronic band structure and the vibrational spectrum of the Type I clathrate “alloy” $\text{Ba}_8\text{Ga}_{16}\text{Ge}_{30-x}\text{Si}_x$ ($1 \leq x \leq 15$). Our calculations show that $\text{Ba}_8\text{Ga}_{16}\text{Si}_{15}\text{Ge}_{15}$ is energetically favored and is a narrow gap semiconductor. The trend in the band gap as function of Si concentration is also presented. The vibrational spectrum indicates low frequency rattling modes caused by Ba atoms that are loosely bound in the Si-Ge framework cages. Such modes may scatter the heat carrying acoustic vibrational modes of the framework, potentially reducing the thermal conductivity.

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Date submitted: 08 Mar 2007

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