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Structural and electronic properties of the germanium-based clathrates Ge_{46} and $Ba8Ge_{46}$ EMMANUEL NENGHABI, CHARLES MYLES, Texas Tech University — Semiconductor clathrates have been of considerable interest in recent years. This is mainly due to structural characteristics that give rise to unique electrical and thermal transport properties. There are two structural clathrate phases, Type I and Type II. Here, we focus on Ge-based Type I clathrates. The Type I structure is simple cubic, with 46 atoms per unit cell. It has 20-atom cages and 24-atom cages combined in a 2 to 6 ratio. The cages can host "guests"; usually alkali or alkaline earth atoms. Using the local density approximation, we have studied the structural and electronic properties of the pristine Type I clathrate Ge_{46} and the Ge clathrate with all cages filled with Ba guests; Ba_8Ge_{46}. The equilibrium lattice structures were obtained by ab initio pseudo potential calculations combined with dynamic minimizations. As found by others [1], the pure Ge_{46} clathrate structure has a slightly higher total energy than that of diamond phase Ge. Further, band structure calculations show that the this material is a semiconductor with a fundamental band gap that is considerably larger than that of the diamond phase. We find that Ba_8Ge_{46} is metallic with the conduction bands slightly modified by the Ba guest atoms in the clathrate cages.

[1] J. Dong and O. F. Sankey, J. Phys: Condens. Matter 11(1999)-6129-6145

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