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First Principles Study of the Properties of the Type II Clathrate Alloy $Si_{136-x}Ge_x$ (x = 8, 32, 96) DONG XUE, CHARLES MYLES, Texas Tech University — The Type-II clathrate materials based on Si, Ge, and Sn have "open-framework" lattices consisting of large "cages" of atoms covalently bonded together. Due primarily to their potential thermoelectric applications, there has been considerable research on these materials with various guest atoms in the cages and with various substitutional atoms on the lattice framework. Also of interest are the pure Type II clathrates M_{136} (M = Si, Ge, Sn) with neither framework substitution nor guest atoms in the cages. A fundamental understanding of the intrinsic properties of these "guest-free" clathrates is therefore also needed. Mixtures or "alloys" of two different Type II clathrate materials are also potentially interesting. For example, Moriguchi *et al.* [1] have reported the successful synthesis of Type II clathrates with mixtures of Si and Ge on the framework lattice. Motivated by these experiments, we have carried out a computational and theoretical study the properties of the Type II clathrate "alloy" $Si_{136-x}Ge_x$. We report the results of DFT-based first-principles calculations of the structural, electronic, vibrational, and thermal properties of $Si_{136-x}Ge_x$ for x = 8, 32, 96. Our calculations have assumed that the ideal lattice symmetry is unaffected by the mixing of Si and Ge. Among other results, we predict that $Si_{136-x}Ge_x$ should have a direct band gap ranging from 1.2 to 2.0 eV. [1]. K. Moriguchi, S. Munetoh, A. Shintani, *Phys. Rev*. B 62, 7138 (2000).

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