

Abstract Submitted
for the TSF15 Meeting of
The American Physical Society

First-Principles

Study of the Structural, Electronic, and Vibrational Properties of the Type-II Clathrate Compounds A_xM_{136} ($A = \text{Na, K, Rb, Cs}$; $M = \text{Si, Ge, Sn}$; $0 \leq x \leq 24$) DONG XUE, CHARLES MYLES, Texas Tech University — Powder X-Ray diffraction (XRD) experiments along with density functional theory (DFT) studies of the Type II clathrate compound $\text{Na}_x\text{Si}_{136}$ have found lattice contraction as the Na content x increases for $0 < x < 8$, and lattice expansion as x increases for $8 < x < 24$. This unusual phenomenon is explained by XRD data which shows that as x increases, the 28-atom Si cages are filled first by Na guests for $x < 8$ and that the 20-atom Si cages are then filled for $x > 8$ [1]. Motivated by this previous work, we have performed a systematic, first-principles computational study of the Type II clathrate compounds A_xM_{136} for $0 \leq x \leq 24$. A is an alkali metal atom. M is Si, Ge, or Sn. Our calculations utilize DFT as implemented in the VASP code. We present results for some structural, electronic and vibrational properties of some of these compounds. Our results include lattice parameters, elastic constants, covalent bond lengths, and electronic state densities. Where possible, our results are compared with experiment. We also show that the low frequency, localized guest vibrational modes can be explained by an avoided crossing effect. These low frequency modes should contribute to a minimization of lattice thermal conductivity. [1] M. Beekman, E.N. Nenghabi, K. Biswas, C.W. Myles, M. Baitinger, Y. Grin, and G.S. Nolas, *Inorganic Chemistry* **49**, 5338 (2010).

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Date submitted: 08 Oct 2015

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