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Theoretical Study of the Properties of the Type II Clathrate A^xSn^{136}, (A = alkali atom; 0 $\leq$ x $\leq$ 24) DONG XUE, CRAIG HIGGINS, CHARLEY MYLES, Texas Tech University — Motivated by recent experimental and theoretical interest in the x dependence of the properties of the Si and Ge-based Type II clathrate materials $A^xSi^{136}$and A^xGe^{136} (A = alkali atom) [1,2] we are carrying out a systematic theoretical study of the properties of the Sn-based Type II clathrate system A^xSn^{136}. Type II clathrates have cage-like lattices in which Si, Ge, or Sn atoms are tetrahedrally-coordinated and sp_3 covalently bonded. The cages can contain "guests"; usually alkali or alkaline earth atoms. These materials are particularly interesting because of their potential use as thermoelectrics. Recent powder X-ray diffraction experiments have found the very interesting result that, for increasing x in the range 0 $\leq$ x $\leq$ 8 a lattice contraction occurs, and that x is increased further (8 $\leq$ x $\leq$ 24), a contrasting lattice expansion results. These observations have motivated us to study the behavior of the lattice constant and other properties as a function of guest concentration in other Type II clathrates. In the present paper, we report preliminary results of a density functional based theoretical study of the properties of K^xSn^{136} as a function of x. We present results for the x dependence of the lattice constant as well as for other structural and electronic properties of this material.

[1] S. Stefanoski and G. Nolas, Cryst. Growth Des. 2011, dx.doi.org/10.1021/cg200756r
[2] M. Beekman, E. Nenghabi, K. Biswas, C. Myles, M. Baitinger, Y. Grin, G.S. Nolas, Inorg. Chem. 49 2010, DOI: 10.1021/ic1005049

Dong Xue
Texas Tech University

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