Theoretical Study of the Properties of the Type II Clathrate A\textsuperscript{x}Sn\textsuperscript{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\textsuperscript{x}Si\textsuperscript{136} and A\textsuperscript{x}Ge\textsuperscript{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\textsuperscript{x}Sn\textsuperscript{136}. Type II clathrates have cage-like lattices in which Si, Ge, or Sn atoms are tetrahedrally-coordinated and sp\textsuperscript{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\textsuperscript{x}Sn\textsuperscript{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.