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Study of the Structural, Electronic, and Vibrational Properties of Some Type-II Sn-Based Clathrates. HENRY STAM, DONG XUE, CHARLES MYLES, Texas Tech University — In addition to the α-Sn and β-Sn crystal structures, Sn can crystallize in the clathrate structures. These contain 20, 24, or 28-atom "cages" which allow for the introduction of loosely bound guest atoms. Due to their low thermal conductivity, some of the Sn-based materials are of interest because of their thermoelectric properties. Motivated by the recent synthesis of the Type II clathrates $K_8Ba_{16}Ga_{40}Sn_{96}$, $Rb_8Ba_{16}Ga_{40}Sn_{96}$, and $Cs_8Ba_{16}Ga_{40}Sn_{96}$ [1, 2], we are performing a systematic, first principles, computational study of the properties of these materials. Our calculations are based on density functional theory and utilize the VASP code. We present results for the structural, electronic and vibrational properties of these compounds. Our predictions include lattice parameters, bulk moduli, electronic densities of states, and vibrational modes. The lattice thermal conductivity and other transport properties of these materials will also be discussed. [1] Schäfer, M. C., Bobev, S.; *J. Am. Chem. Soc.* 135, 1696 (2013) [2] Koda, S., Kishimoto, K., Akai, K., Asada, H., Koyanagi, T.; *J. Appl. Phys.*116, 023710 (2014)

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