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First-Principles Study of the Structural, Vibrational and Thermal Properties of Some Type II Tin-Based Clathrates HADEEL ZAHID, DONG XUE, CHARLEY 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 the introduction of loosely bound guest atoms. Due to their low thermal conductivity, some of the Sn-based materials are of interest because as possible thermoelectric materials. Here, we report the results of a systematic, first principles, computational study of the properties of some type II Sn-based clathrate materials. This study was motivated by a recent computational study [1] of the properties of the Type-II clathrate compounds A_xSi_{136} and A_xGe_{136} (A=Na, K, Rb, Cs; $0 \leq x \leq 24$), which increased the understanding of the role of the guest atoms and their composition x in determining the properties of the clathrate materials. Our calculations are based on density functional theory and utilize the VASP code. We present results for the structural, vibrational, and thermal properties of the Type II clathrates $Sn_{136,}$ and A_xSn_{136} (A = Na, K, Cs; x = 8, 16, 24). Our predictions include lattice parameters, elastic constants, sound velocities, vibrational modes, and thermal properties. The predicted dependences of these properties both on the guest atom composition x and on the choice of guest atom are discussed. [1] D. Xue, C. Myles, C. Higgins; Materials 2016, **9**(8), 691.

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