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Theoretical Study of the Properties of the Type II Clathrates A_xB_{136}(A=alkali atom;B=Si,Ge,Sn0 $\leq$ x $\leq$ 24) DONG XUE, CRAIG HIGGINS, CHARLEY MYLES[1], Department of Physics, Texas Tech University — Type II clathrate semiconductors have cage-like lattices in which Group IV atoms are tetrahedrally-coordinated and sp^3 covalently bonded. The cages can contain "guest" atoms; usually alkali or alkaline earth atoms. These materials are of interest because of their thermoelectric properties. Motivated by recent experimental and theoretical interest [1,2] in the x dependence of properties of the Si and Ge-based Type II clathrate materials A_xSi_{136} and A_xGe_{136} (A = alkali atom) we are carrying out a systematic theoretical study of the properties of the Type II clathrate systems A_xB_{136}(A = alkali atom; B = Si, Ge, Sn). Recent powder X-ray diffraction experiments have found the very interesting result that in Na_xSi_{136}, for increasing x in the range $0 \leq x \leq 8$ a lattice contraction occurs and that as 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 several Type II clathrates. We present results of a density functional based study of the properties of A_xB_{136} as a function of x. Results are discussed for the x dependence of the lattice constant and for other structural and electronic properties of these materials. [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

[1]Dr. Charley W. Myles is the professor of Physics Department at Texas Tech University.

Dong Xue
Department of Physics, Texas Tech University

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