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Theoretical Study of the Properties of the Type II Clathrates $\mathbf{A}_x\mathbf{Si}_{136}$ and $\mathbf{A}_x\mathbf{Ge}_{136}$ (A = Na, K) CRAIG HIGGINS, Texas Tech University, CHARLEY MYLES, Professor, Texas Tech University, TEXAS TECH TEAM — Type II clathrate semiconductors have cage-like lattices where atoms are tetrahedrally coordinated and sp^3 bonded. An observed property of these materials is the variation of unit cell volume as different types of alkali metal atoms are placed in the clathrate cages. Experiments[1] on Na_xSi_{136} reveal that, starting with Si_{136}, as x increases ($0 < x < 8$), the cell volume contracts; where ($8 < x < 24$), the cell volume expands. This variation with x has been explained[2] as due to preferential incorporation of Na into the Si_{28} cages for $x < 8$, followed by incorporation into the Si_{20} cages for $8 < x$ (when all Si_{28} cages are full). With this motivation, we have used density functional theory to explore the possibility Type II Si and Ge clathrates with alkali atom guests other than Na may exhibit a similar variation in cell volume with guest inclusion. We present results for the electronic and vibrational properties of the Na_xSi_{136}, Na_xGe_{136}, K_xSi_{136}, and K_xGe_{136} clathrates. These results are compared with experiment and the properties of the materials are compared and contrasted.

[1]M. Beekman, et al, *Inorganic Chem* 49, 5338 (2010)
[2]Ibid.

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