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Theoretical Study of the Structural and Electronic Properties of K_xSi_{136}, (x = 1, 8, 18) CRAIG HIGGINS, CHARLES MYLES, Texas Tech University, TEXAS TECH TEAM — 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. Measurements of the lattice constant [1] as a function of Na concentration x in Na_xSi_{136} ($0 \leq x \leq 24$) have shown the interesting property that, as x is increased in the range ($0 \leq x \leq 8$), the lattice constant decreases and that as x is increased further in the range ($8 \leq x \leq 24$), the lattice constant increases. We note that some measurements of the properties of $K_{17.8}Si_{136}$have also recently been reported [2]. 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 the results of a theoretical study of the properties of K_xSi_{136} as a function of x. We have used density functional theory to investigate the properties of this material with guest concentrations of x = 1, 8, and 18. Our results show that, similar to previous results for Na_xSi_{136}, the lattice constant as a function of x has a minimum at x = 8. We also report results for other structural and electronic properties of K_xSi_{136}.

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[2] S. Stefanoski and G. Nolas, Cryst. Growth Des. 2011, dx.doi.org/10.1021/cg200756r

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