Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

First-Principles Computational Study of the Properties of the Clathrate Compounds $A_8Al_8Si_{128}$ (A=Na,Rb,Cs) DONG XUE, CHARLES MYLES, Texas Tech University — Our recent study [1] of the properties of the Type-II binary clathrate compounds A_xSi_{136}, A_xGe_{136} and A_xSn_{136} (A=Na, K, Rb, Cs; $0 \leq x \leq 24$) has increased the understanding of the role of the guest atoms and their composition x in determining the properties of these materials. For Na_xSi_{136}, our results have helped to explain the observed dependence of the lattice constant on x, which has a very unusual, distinct minimum at x = 8. In this case, we have also found a "Mexican-hat" shaped effective potential curve for the Na atom motion in the large, (28-atom) Si cages. Motivated by these fascinating results for Na_xSi_{136}, we have extended our study of the effects of alkali guests on the properties of the Type-II clathrates to include their effects on the properties of the Type-II the ternary clathrate compounds $A_8Al_8Si_{128}$ (A=Na,Rb,Cs). An earlier study of similar compounds, $(Rb,Cs)_8Ga_8Si_{128}$, has found low frequency guest rattling modes (~41-51 cm^{-1}). Here, we report the results of a first-principles computational study of the electronic, structural and vibrational properties of the compounds $A_8Al_8Si_{128}$ (A=Na,Rb,Cs). We contrast our results with those for $(Rb,Cs)_8Ga_8Si_{128}$, as well as with our recent results for the binary clathrates A_xSi_{136} (A=Na,Rb,Cs). Our calculations are based on the Local Density Approximation to Density Functional Theory, as implemented by the VASP code. [1] D. Xue, C. Myles, C. Higgins; Materials 2016, **9**(8), 691.

Charles Myles
Texas Tech University

Date submitted: 11 Nov 2016 Electronic form version 1.4