Abstract Submitted for the MAR11 Meeting of The American Physical Society

First Principles Studies of the Thermoelectric Figure of Merit of Zintl Compounds $Ca_{14}AlSb_{11-x}As_x$ TRINH VO, PAUL VON ALLMEN, JEAN-PIERRE FLEURIAL, Jet Propulsion Lab, CalTech — We present predictions for the thermoelectric Figure of merit (ZT) of zintl compounds $Ca_{14}AlSb_{1-x}As_x$ obtained from Density Functional Theory calculations. The Seebeck coefficient, S, was obtained using the Boltzmann transport equation in the relaxation time approximation and first principles electronic structure calculations. We found that the Seebeck coefficient changes dramatically when one or more Sb atoms in the zintl compound $Ca_{14}AlSb_{11}$ are replaced with one or more As atoms, and that the difference in S between the original $Ca_{14}AlSb_{11}$ and the substituted one, $Ca_{14}AlSb_{11-x}As_x$, depends strongly on the positions of substituting As atoms.

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Date submitted: 17 Nov 2010

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