Abstract Submitted
for the SES16 Meeting of
The American Physical Society

Entropy of Exciton Formation in 2D Atomic Layer Transition Metal Dichalcogenides QUINTON RICE, TIKARAM NEUPANE, DULITHA JAYAKODIGE, BAGHER TABIBI, FELIX SEO, Hampton University — The 2-dimensional atomic layer transition metal dichalcogenides (TMDCs, MX_2; M=Mo or W; X=S, Se, or Te) are of special importance for optoelectronic applications because of the structural tunability of bandgaps in visible and near-infrared regions and the bandgap crossover from direct (monolayer) to indirect (bilayer or multilayer). The role of the acoustic phonon energy and electron-phonon coupling which is critical to the formation of excitons is investigated using the O'Donnell and Chen relation for temperature-dependent bandgaps of semiconductors. The change in entropy of exciton formation is given by the derivative of the O'Donnell and Chen relation when the bandgap energy is the standard Gibbs free energy. The analysis suggests the change in entropy of exciton formation with higher energy phonons (100 meV) is constant until 90 K while lower energy phonons (10 meV) approaches a constant value of $-2Sk_B$ between 250 K and 300 K where$S$is the strength of electron-phonon interaction and $k_B$is the Boltzmann constant. Increased scattering and spontaneous decay probabilities of higher energy phonons may result from the larger electron-phonon interaction of less energetic phonons. A ˜3-fold increase in the change in entropy of exciton formation was observed while the electron-phonon coupling strength largely determines the bandgap energy compared to the average acoustic phonon energy. Acknowledgement: This work at HU is supported by ARO W911NF-15-1-0535, NSF HRD-1137747, and NASA NNX15AQ03A.

Quinton Rice
Hampton University

Date submitted: 14 Oct 2016 Electronic form version 1.4