Abstract Submitted for the MAR13 Meeting of The American Physical Society

Raman spectroscopy of single layer graphitic carbon nitride JOEL THERRIEN, YANCEN LI, ECE Dept UMass Lowell, DANIEL SCHMIDT, Plastics Engineering Dept UMass Lowell, ADAM COLLARD, Physics U. Texas Austin, DANIEL FINKENSTADT, TAYLOR YUST, US Naval Acdemy — Single layer graphitic carbon nitride (referred to as melon) has been synthesized by our group in sizes up to 50  $\mu$ m across. Raman spectroscopy has been performed on single layer melon and multi layer samples. Much like graphene, melon shows a unique raman spectrum when in single layer form. These experimental results have been compared to theoretical calculations for possible melon structures. Bond counts for feasible structures of hexagonal carbon nitride have been calculated and some possible structures have been eliminated from consideration based on these efforts. Periodic supercells have been built to make sheets based on structures to be modeled via density-functional theory, as implemented using VASP, to calculate thermodynamic and structural stability and frequencies of IR and Raman active modes.

Joel Therrien ECE Dept UMass Lowell

Date submitted: 09 Nov 2012

Electronic form version 1.4