Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Theoretical and Experimental Studies of Designed Molecular Interfaces for Improved Thermal Conductivity[1] ALEX KERR, KIERAN MULLEN, Homer L. Dodge Dept. of Physics and Astronomy, DANIEL GLATZHOFER, MATTHEW HOUCK, Department of Chemistry and Biochemistry, University of Oklahoma, PAUL HUANG, School of Chemical, Biological Materials Engineering, University of Oklahoma — Certain molecular structures such as carbon nanotubes (CNTs) can potentially improve the thermal conductivity of composite materials. However, their thermal boundary resistance is an obstacle to their effective implementation as a medium for heat flow. We are concerned with overcoming this Kapitza resistance with the aid of chemical functional groups. These functional groups will, in principal, eliminate phonon mismatch between our structures and their matrix. The result will maximize the transmission of thermal vibrations to and from their surrounding medium. We develop a method to predict the thermal properties of our functionalized materials through the calculation of vibrational normal modes and Green's functions. We show how the configuration of attached functional groups affect the samples' thermal conductivity (κ) and attempt to find the arrangement in which κ is maximized. We will make explicit comparisons with thermal conductivity experiments done on nanocomposites of functionalized and pristine CNTs. We will discuss how the bonds connecting the functional groups to the CNT affects κ. We compare these results to measurements on our particular synthesized materials and discuss how to better optimize their design.

[1]This work was supported by supported by NSF grant DMR-1310407.

Kieran Mullen
Homer L. Dodge Dept. of Physics and Astronomy

Date submitted: 06 Nov 2015 Electronic form version 1.4