Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

**Molecular Dynamical Simulation of Thermal Conductivity in Amorphous Structures**[1] FREDDY DEANGELIS, ASEGUN HENRY, Georgia Inst of Tech — While current descriptions of thermal transport exists for well-ordered materials such as crystal latices, new methods are needed to describe thermal transport in disordered materials, including amorphous solids. Because such structures lack periodic, long-range order, a group velocity cannot be defined for thermal modes of vibration; thus, the phonon gas model cannot be applied to these structures. Instead, a new framework must be applied to analyze such materials. Using a combination of density functional theory and molecular dynamics, we have analyzed thermal transport in amorphous structures, chiefly amorphous germanium. The analysis allows us to categorize vibrational modes as propagons, diffusons, or locons, and to determine how they contribute to thermal conductivity within amorphous structures. This method is also being extended to other disordered structures such as amorphous polymers.

[1]This material is based upon work supported by the National Science Foundation Graduate Research Fellowship Program under Grant No. DGE-1148903.

Freddy DeAngelis
Georgia Inst of Tech

Date submitted: 11 Nov 2016 Electronic form version 1.4