

Abstract Submitted  
for the OSF17 Meeting of  
The American Physical Society

**Phonon Dispersion and Thermal Conductivity of Carbon Nanotubes (CNTs)** TUAN LE, MAHFUZA KHATUN, Ball State University — We will present phonon dispersion, phonon density of states, and thermal conductivity of carbon nanotubes (CNTs). These one-dimensional carbon nanotubes are extremely versatile and robust with their high electrical and thermal conductivities, and mechanical strengths. The theoretical analyses for the phonon dispersion relation and density of states are based on Dynamical Matrix method. The thermal conductivity and heat flux autocorrelation function are obtained using Green–Kubo formalism. The Nose Hoover thermostat and the Tersoff interatomic potential are incorporated in the simulator. Three open source code have been used in this investigation. These include: Visual Molecular Dynamics (VMD), Dynamical Matrix Code, and the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS). The numerical computation for thermal conductivity is based on equilibrium molecular dynamics (EMD) technique. Results of CNTs with different chirality, length, and temperature will be discussed.

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Date submitted: 12 Sep 2017

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