~~Thermal management engineering depends critically on accurate predictions of the vibrational mode properties.~~ The mode properties allow for a deeper understanding of the nature of thermal transport at the atomistic scale. ~~The properties can be used to understand the effects of vibrational scattering mechanisms in bulk and nanostructured materials.~~

Thermal transport in ~~ordered~~ (crystalline) materials is well understood in terms of the phonon gas model. Disordering a crystal (i.e., alloying, amorphization) breaks down the phonon gas theory and ~~a new~~ theoretical formulation is necessary. Typical ~~theoretical~~ formulations begin with perturbation theory, which is only valid for weakly disordered systems. These perturbation theories lead to simple models ~~which~~ can be fit empirically to experimental measurements, but lack predictive capabilities. Predictive methods ~~which~~ do not rely on perturbation theory are still in ~~active~~ development, ~~where the thermal conductivity and the vibrational mode properties are desired. To asses the predictive capabilities of the theoretical models for thermal transport in disordered materials requires a comprehensive study of the vibrational mode properties in a range of disordered materials.~~

The vibrational mode properties of crystalline, alloyed, and amorphous materials are studied ~~in this work~~ using ~~several~~ predictive methods. Because disordering complicates the theory of thermal transport, each predictive method provides complimentary information ~~which~~ is compared wherever possible. ~~By comparison, critical information about the vibrational mode properties is identified.~~ Important assumptions about the nature of thermal transport in disordered materials are investigated using fully atomistic models. The predicted results are compared to experimental measurements, perturbative methods, and phenomenological/empirical models. The results presented in this work provide a theoretical and computational framework for the study of emerging disordered and nanoscaled materials.