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Prediction of vibration modes and thermal conductivity for amorphous ZnO-based materials YU-TING CHENG, ANINDYA ROY, MICHAEL L. FALK, Johns Hopkins University — Amorphous materials, due to their distinct physical and chemical properties, have been widely used in photovoltaics, thermoelectrics and integrated circuits. Because the thermal conductivity is critical to the performance of such devices, the thermal transport in amorphous materials has received considerable attention in the last decade. So far, a number of experimental studies and theoretical models have reported the vibration modes and thermal conductivities for amorphous Si and SiO_2. However, the applicability of these vibration mode analyses and thermal conductivity models for other amorphous materials has not been studied. In this work, we employ the molecular dynamics (MD) simulations and Allen-Feldman (AF) theory [1] to investigate the vibration modes and thermal conductivity of amorphous ZnO-based materials. ZnO is basis of a promising class of n-type semiconductors for thermoelectric application. Additionally, from this work, the contribution of individual vibrational modes to the thermal conductivity can be characterized. These results are expected to guide the interpretation of thermal transport in amorphous ZnO-based materials and the optimization for their performance with different applications. [1] P. B. Allen and J. L. Feldman, Phys. Rev. B **48**, 12581 (1993).

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