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A first principles method for simulating phonons in strongly disordered materials TOM BERLIJN, OLIVIER DELAIRE, BEN LARSON, Oak Ridge National Laboratory — At the microscopic level the flow of vibrational heat is encoded not only in the energies of phonons but also in their lifetimes. In many functional materials these phonon lifetimes are controlled by strong disorder. Such systems are difficult to understand from conventional perturbation theories or mean field treatments. Here we will present an affordable and accurate first principles method for simulating phonons in strongly disordered materials. The method will be illustrated with applications ranging from thermoelectrics to nuclear fuels. TB was supported as a Wigner Fellow at the Oak Ridge National Laboratory, OD was supported by the US DOE-BES, Materials Science and Engineering Division, and BL was supported by the CMSNF Energy Frontier Research Center.

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