Calculation of energy relaxation rates of fast particles by phonons in crystals\textsuperscript{1} MICAH PRANGE, LUKE CAMPBELL, DANGXIN WU, SEBASTIEN KERISIT, Pacific Northwest National Laboratory — We present \textit{ab initio} calculations of the temperature-dependent exchange of energy between a classical charged point-particle and the phonons of a crystalline material. The phonons, which are computed using density functional perturbation theory (DFPT) methods, interact with the moving particle via the Coulomb interaction between the density induced in the material by phonon excitation and the charge of the classical particle. Energy relaxation rates are computed using time-dependent perturbation theory. The method, which is applicable wherever DFPT is, is illustrated with results for several important scintillators whose performance is affected by electron thermalization. We discuss the influence of the form assumed for quasiparticle dispersion on theoretical estimates of electron cooling rates.

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