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Phonon-Assisted Auger Recombination in Medium and Wide Band-Gap Materials from First Principles[1] DANIEL STEIAUF, Materials Department, University of California, Santa Barbara, EMMANOUIL KIOUPAKIS, Materials Science and Engineering, University of Michigan, Ann Arbor, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara — GaN and GaAs and their alloys are technologically important materials for solid-state optoelectronic devices such as LEDs and lasers. The internal quantum efficiency of these devices, defined as the fraction of electron-hole pairs converted to photons, is limited by nonradiative loss mechanisms. Auger recombination is such a mechanism which limits the efficiency at high carrier densities. The energy and momentum of an electron-hole pair is transferred to a third carrier instead of creating a photon. We present state-of-the-art results of first-principles calculations of the Auger recombination rate coefficients both for the simple direct purely Coulombic process and the indirect phonon-assisted process. We find the absolute values of these recombination rates as well as their relative importance. In GaAs, when energy and momentum of the recombining pair are transferred to an Auger electron, the phonon-assisted process is several orders of magnitude stronger than the direct process, while for recombinations that create an Auger hole, the direct and phonon-assisted processes contribute almost equally. For lower band gaps, the electron processes become equally strong, and also the direct process becomes comparable in magnitude.

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