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Auger recombination in gallium arsenide from first principles[1] DANIEL STEIAUF, Materials Department, University of California, Santa Barbara, EMMANOUIL KIOUPAKIS, Materials Department, UC Santa Barbara; Materials Science and Engineering, University of Michigan, Ann Arbor, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara — GaAs and its 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 loss mechanisms. Of particular importance at high carrier densities is Auger recombination, a non-radiative process where the energy and momentum of the recombining electron-hole pair is transferred to a third carrier. Here we use density functional theory to study Auger recombination in GaAs from first principles. When considering Auger recombination due to Coulomb interaction only, the calculated rate is too small and cannot account for the experimental observations. However, once additional electron-phonon interactions are included, the theoretical recombination rate increases towards the experimental value. Our work provides insight into the microscopic origins of the loss in III-V LEDs at high injected-carrier densities, and in the mechanisms governing Auger recombination rates in general.

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