

Accurate first principles detailed balance determination of Auger recombination and impact ionization rates in semiconductors

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The technologically important problem of predicting Auger recombination lifetimes in semiconductors is addressed by means of a fully first-principles formalism¹. The calculations employ highly precise energy bands and wave functions provided by the full-potential linearized augmented plane wave (FLAPW) code based on the screened exchange local density approximation. The minority carrier Auger lifetime is determined by two closely related approaches: *i*) a direct evaluation of the Auger rates within Fermi's Golden Rule, and *ii*) an indirect evaluation, based on a detailed balance formulation combining Auger recombination and its inverse process, impact ionization, in a unified framework. Calculated carrier lifetimes determined with the direct and indirect methods show excellent consistency *i*) between them for *n*-doped GaAs and *ii*) with measured values for GaAs and InGaAs. This demonstrates the validity and accuracy of the computational formalism for the Auger lifetime and indicates a new sensitive tool for possible use in materials performance optimization.

¹S.Picozzi, R.Asahi, C.B. Geller and A.J.Freeman, Phys. Rev. Lett. **89**, 197601 (2002).