Noneradiative hot carrier capture cross section of defects in GaN from first principles

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Recent progress in first-principles calculations of multiphonon processes in solids[1,2] allows direct calculation of nonradiative hot-carrier capture cross sections of defects in semiconductors. We apply the computational method in[1] to electron and hole capture cross sections of defects in GaN. As formulated, the method contains zeroth-order matrix elements for the phonon-assisted electron (or hole) transition, whose contribution is expected to be larger than the contributions of the usual, first-order, electron-phonon coupling matrix elements[2]. The calculated cross sections are compared to the first-order results in[2] and to experiments.

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