Abstract Submitted
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First-Principles Calculation of Carrier Lifetimes in Semiconductors[1] VINCENZO LORDI, PAUL ERHART, DANIEL ABERG, Lawrence Livermore National Lab, Livermore, CA — We have developed first-principles methods based on density functional theory to calculate carrier lifetimes in semiconductors related to trapping on deep-level defects. Lifetimes are determined based on Schottky-Read-Hall theory, using recombination rates calculated from first principles for several possible, competing mechanisms: radiative recombination, phonon-assisted (nonradiative) recombination, and Auger recombination. The recombination rates are calculated within a fully first-principles framework with no empirical parameters. We have recently applied these methods to study the role of native and impurity defects in reducing carrier lifetimes in bulk single-crystal aluminum antimonide (AlSb) and cadmium telluride (CdTe), two promising materials for high-resolution room-temperature gamma radiation detection.

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