Abstract Submitted
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Auger recombination in scintillator materials from first principles[1] ANDREW MCALLISTER, EMMANOUIL KIOUPAKIS, University of Michigan, DANIEL ÅBERG, Lawrence Livermore National Laboratory, ANDRÉ SCHLEIFE, University of Illinois at Urbana-Champaign — Scintillators convert high energy radiation into lower energy photons which are easier to detect and analyze. One of the uses of these devices is identifying radioactive materials being transported across national borders. However, scintillating materials have a non-proportional light yield in response to incident radiation, which makes this task difficult. One possible cause of the non-proportional light yield is non-radiative Auger recombination. Auger recombination can occur in two ways - direct and phonon-assisted. We have studied both types of Auger recombination from first principles in the common scintillating material sodium iodide. Our results indicate that the phonon-assisted process, assisted primarily by short-range optical phonons, dominates the direct process. The corresponding Auger coefficients are $5.6 \pm 0.3 \times 10^{-32}\text{cm}^6\text{s}^{-1}$ for the phonon-assisted process versus $1.17 \pm 0.01 \times 10^{-33}\text{cm}^6\text{s}^{-1}$ for the direct process. At higher electronic temperatures the direct Auger recombination rate increases but remains lower than the phonon-assisted rate.

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