Transport of Hot Electrons in Scintillators: NaI and SrI_2

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The hot electrons induced by incident gamma-ray in scintillators lose their energy from one energy gap (EG) above to conduction band minimum (CBM) though various scattering channels, among which the most important one is phonon scattering [1]. Hence, the transport of hot electrons should be characterized by mainly their group velocities and optical phonon energies. We present results for a density functional theory study of the electron group velocities of two halide scintillators: NaI and SrI_2. The holes in both materials are accepted to self-trap less than several picoseconds, forming a core of self-trapped holes (STH) with a radius of about 3nm. It is demonstrated that the inclusion of full band structure significantly improves the result with respect to the prediction of a free electron gas model. A recent model of quenching and transport showed that linear quenching by trapping on defects affects the both light yield and nonproportionality of scintillators [2]. Our calculation shows that the average group velocity of NaI is about 5 times greater than that of SrI_2. Taking their similar optical phonon energies into consideration, we expect that the hot electrons in NaI cover a much bigger range in space through transport before thermalization. Therefore, we expect greater chance of getting trapped on deep defects for the thermalized electrons of NaI during their hopping walk back toward the STH core for recombination, which causes less relative light yield and more nonproportionality. Furthermore, we deduce that this tread can be generalized to explain the performance of two different scintillator material families: monovalent halides which in general have simple unit cells and bigger group velocities and multivalent halides which in general have relatively complicated unit cells and smaller group velocities. These results suggest a design parameter for scintillator materials.

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