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First-principles calculations of self-trapping of carriers and excitons in NaI and SrI_2

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While the general potential of scintillators as radiation detectors has been demonstrated, one of the current goals is to develop materials with improved energy resolution sufficient to detect fissile materials with a low probability of errors at ports, borders, and airports. The poor resolution has been linked to the non-linear response to the gamma ray energy. Fundamental understanding of this requires detailed knowledge of elementary electronic excitation processes. In particular, in most metal halide scintillators charge carriers and excitations localize and create self-trapped species associated with large effective masses and slow diffusivities. First-principles modeling is essential for providing quantitative understanding of the involved microscopic processes. Here, we present comprehensive ab-initio calculations, with techniques ranging from hybrid DFT+exact exchange to self-consistent GW and Bethe-Salpeter approach, for modeling the electronic structure and mobilities of self-trapped carriers and excitons in metal halides with particular attention given to sodium and strontium iodide.