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Electronic band structure of lanthanum bromide and strontium iodide from many-body perturbation theory calculations¹

DANIEL ABERG, Lawrence Livermore National Laboratory, PAUL EHART, Chalmers University of Technology, BABAK SADIGH, Lawrence Livermore National Laboratory — Rare-earth based scintillators represent a challenging class of scintillator materials due to pronounced spin-orbit coupling and subtle interactions between d and f states that cannot be reproduced by standard electronic structure methods such as density functional theory. In this contribution we present a detailed investigation of the electronic band structure of LaBr_3 using the quasi-particle self-consistent GW (QPscGW) method. This parameter-free approach is shown to yield an excellent description of the electronic structure of LaBr_3 . Specifically we reproduce the correct level ordering and spacing of the 4f and 5d states, which are inverted with respect to the free La atom, the band gap as well as the spin-orbit splitting of La-derived states. We furthermore present electronic structure calculations using G_0W_0 for the important scintillator material SrI_2 . We explicitly take into account spin-orbit coupling at all levels of the theory. Our results demonstrate the applicability and reliability of the GW approach for rare-earth halides and complex halides. They furthermore provide an excellent starting point for investigating the electronic structure of rare-earth dopants such as Ce and Er.

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