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Ab-Initio analysis of TlBr: limiting the ionic current without degrading the electronic one CEDRIC ROCHA LEAO, VINCENZO LORDI, Lawrence Livermore National Lab — Although TlBr in principle presents all the theoretical requirements for making high resolution room temperature radiation detectors, practical applications of TlBr have proven to be nonviable due to the polarization that is observed in the crystal after relatively short periods of operation. This polarization, that is believed to be caused by accumulation of oppositely charged ionic species at the ends of the crystal, results in an electric field that opposes that of the applied bias, counter-acting its effect. In this work, we use state of the art quantum modeling to benchmark the theoretical limits for the performance of TlBr as a radiation detector, showing that the best experimental reports demonstrate near-ideal electronic characteristics. We then propose a model to inhibit the detrimental ionic current in the material without impacting the excellent properties of the electronic current. Prepared by LLNL under Contract DE-AC52-07NA27344.

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