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First-principle Calculations of Donor and Acceptor Levels in PbI2 for Ultra-fast Scintillation GAIGONG ZHANG, Program in Applied Science, UC Davis, ANDREW CANNING[1], Computational Research Division, LBNL, NIELS GRONBECH-JENSEN[2], Program in Applied Science, UC Davis, LIN-WANG WANG, Materials Sciences Division, LBNL, STEPHEN DERENZO, Life Sciences Division, LBNL — In the past PbI2 was studied as a candidate for semi-conductor gamma ray detectors as well as more recently as an ultra-fast scintillator for time-of-flight applications. The ultra-fast scintillation properties of this materials are believed to be related to donor-acceptor recombination in both the pure and doped system. This work presents first-principles electronic structure calculations of donor and acceptor levels for intrinsic defects and doped impurities in PbI2. We performed density functional theory calculations within the generalized gradient approximation with U correction for the donor and acceptor modeling. For a more accurate description of band gaps and structures, we used more advanced methods, such as GW. Our study shows that intrinsic defects significantly affect the luminescence properties of bulk PbI2. Moreover, the relative position of intrinsic defect levels to doped impurity levels can influence the luminosity. We will compare our theoretical work to known experimental work for this material.

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