

Abstract Submitted  
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**Electronic Structure Study of Cerium Doped Scintillators**<sup>1</sup> DA GAO, MICHAEL MCILWAIN, Idaho National Laboratory — The interest shown in recent years related to cerium doped lanthanum halides, such as LaCl<sub>3</sub>, LaBr<sub>3</sub>, and LaI<sub>3</sub>, is mainly due to their potential applicability as gamma ray scintillation detectors. We have performed a comprehensive theoretical study of these materials to better understand the scintillation process and define the nature of the self trapped exciton (STE) associated with thermally dependent scintillation process. The present work focuses on the study of the luminescence properties of cerium doped lanthanum halide scintillators from the point view of solid state band structure calculations. Our calculated band structures are in good agreement with experimental values. For example, LaCl<sub>3</sub> band gap is calculated to be 6.85 eV as compared to approximately 7.0 eV for the experimentally determined value. The theoretically calculated excitation spectra are also compared with the experimental spectra. We find that scintillation efficiencies are dependent on the location of the of Ce<sup>3+</sup> ground 4f and excited 5d levels with respect to the fundamental band gap of the host materials.

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