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Electronic Structure Studies of Ce-doped Gamma Detector Materials ANDREW CANNING, Computational Research Division, Lawrence Berkeley National Laboratory , ROSTYSLAV BOUTCHKO, STEPHEN DERENZO, Life Sciences Division, LBNL , LIN-WANG WANG, Computational Research Division, LBNL, MARV WEBER, Life Sciences Division, LBNL — Cerium doped materials such as the Lanthanum Halides represent some of the brightest known scintillators for the detection of gamma rays. The scintillation process in Cerium doped materials corresponds to the transition from a 5d to 4f state on the Cerium atom where the 5d and 4f states must lie in the gap of the host materials. We have performed electronic structure calculations for many different Cerium doped materials using density functional based methods to determine the positions of the 5d and 4f states relative to the valence and conduction bands of the host materials. We find good agreement with experimental results for the systems studied in particular for the Lanthanum Halides. Our theoretical calculations will be used as a first step screening for candidate new detector materials. This work is funded by the Dept. of Homeland Security, Domestic Nuclear Detection Office.

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