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First-principles studies of Ce and Eu doped inorganic materials as candidates for scintillator gamma ray detectors¹ ANDREW CANNING, Lawrence Berkeley National Laboratory, UC Davis , SLIM CHOUROU, STEPHEN DERENZO, Lawrence Berkeley National Laboratory — We have performed high-throughput DFT based (GGA+U) band structure calculations for new Ce and Eu doped wide band gap inorganic materials to determine their potential as candidates for gamma ray scintillator detectors. These calculations are based on determining the 4f ground state level of the Ce and Eu relative to the valence band of the host as well as the position of the Ce and Eu 5d excited state relative to the conduction band of the host. We find many classes of candidate materials where the 5d is in the conduction band preventing scintillation. Even when the Eu and Ce 4f and 5d levels are placed well in the gap of the host, traps on the host can also prevent the energy of the gamma ray transferring to the Eu or Ce. We therefore also performed calculations for host hole traps and electron traps to compare their energies to the Ce and Eu 4f and 5d levels.

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