

Abstract Submitted  
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**First-principles studies of Ce and Eu doped inorganic scintillator gamma ray detectors**<sup>1</sup> ANDREW CANNING, ANURAG CHAUDHRY, Lawrence Berkeley National Laboratory, UC Davis, ROSTYSLAV BOUTCHKO, STEPHEN DERENZO, Lawrence Berkeley National Laboratory — We have performed DFT based 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. Host hole and electron traps as well as STEs (self trapped excitons) can also limit the transfer of energy from the host to the Ce or Eu site and therefore limit the light output. We also present calculations for host hole traps and STEs to compare the energies to the Ce and Eu excited states.

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Andrew Canning  
Lawrence Berkeley National Laboratory, UC Davis

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